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Ballistic conductance of a quantum sphere

J. Brüning†, V. A. Geyler‡, *V. A. Margulis*‡ and M. A. Pyataev‡
† Institut für Mathematik, Humboldt-Universität zu Berlin,
Unter den Linden 6, D-10099 Berlin, Germany
‡ Institute of Physics and Chemistry, Mordovian State University,
430000, Saransk, Russia

Abstract. The conductance of a quantum sphere with two one-dimensional wires attached to it is investigated. An explicit form for the conductance as a function of the chemical potential is found from the first principles. The form and positions of the resonance maxima on the plot of the conductance are studied.

Introduction

The aim of this paper is the theoretical study of the ballistic electron transport of a nanodevice consisting of a sphere and two wires attached to the sphere. We consider an idealized model in which the wires are taken to be one-dimensional. This crucial simplification is based on the possibility to describe the electron motion in nanowires only by means of longitudinal part of wave functions. To join the wave functions in the wires with those in the sphere we use boundary conditions at points of gluing the wires to the sphere. These boundary conditions are similar to those in the zero-range potential theory and lead to appearance of phenomenological parameters like the scattering length for a zero-range potential [ ]. A useful mathematical formalization of the approach considered here is founded on the Krein resolvent formula from the self-adjoint operator theory and gives the scattering matrix in terms of the renormalized Green functions for the free Hamiltonians on the sphere and in the wires.

1. Boundary conditions and scattering matrix

We consider a wire $\mathbf{R}_j^+$ $(j = 1, 2)$ as the semi-axis $x \geq 0$. The wire $\mathbf{R}_j^+$ is attached to the sphere $\mathbf{S}$ ($\mathbf{S}$ has the radius R) by gluing the point 0 from $\mathbf{R}_j^+$ to a point q_j from $\mathbf{S}$. Denote by H_0 the electron Hamiltonian on $\mathbf{S}$, which coincides with $(2m^*R^2)^{-1}\mathbf{L}^2$, where $\mathbf{L}$ is the angular momentum operator and m^* is the effective mass. A wave function f of the device consists of three parts: f_0, f_1, f_2, where f_0 is a function on $\mathbf{S}$, and f_j $(j = 1, 2)$ is a function on $\mathbf{R}_j^+$. Let $r(q, q')$ be the geodesic distance between points q and q' on the sphere $\mathbf{S}$. Since we are going to use boundary conditions of the zero-range potential theory, we must consider the function f_0 having the following asymptotics near the points q_j [ ]:

$$f_0(x) = a_j(f_0) \ln r(x, q_j) + b_j(f_0) + o(1), \tag{1}$$

where $a_j(f_0)$ and $b_j(f_0)$ are complex numbers; they play the role of the boundary values for the function f_0. As to the functions f_j, the role of their boundary values are played, as usual, by $f_j(0)$ and $f_j'(0)$. For reasons of space we shall consider here only the boundary

conditions of the Neumann type; the most general form of these conditions is given by the expressions

$$\begin{cases} b_j(f_0) = \sum\limits_{k=1}^{2} \left[\beta_{jk} a_k(f_0) + \alpha_{jk} f_k(0)\right], \\ f_j'(0) = \sum\limits_{k=1}^{2} \left[\tilde{\alpha}_{jk} a_k(f_0) + \gamma_{jk} f_k(0)\right]. \end{cases} \tag{2}$$

Here the parameters α_{jk}, β_{jk} and γ_{jk} forms 2×2-matrices A, B, and C, respectively, such that the 4×4-matrix

$$P = \begin{bmatrix} B & A \\ A^* & C \end{bmatrix}$$

is Hermitian. Let $\widetilde{G}_0(q, q'; E)$ be the renormalized Green function of H_0, i.e., the function obtained from the Green function $G_0(q, q'; E)$ by extracting the singular term $(m^* R^2/\pi\hbar^2) \ln r(q, q',)$. Denote by $Q_0(E)$ the Krein $\mathcal{Q}$-matrix [ ]; this is a matrix with the elements $Q_0^{jk}(E) = G_0(q_j, q_k; E)$, if $j \neq k$, and $Q_0^{jk}(E) = \widetilde{G}_0(q_j, q_k; E)$, if $j = k$. Using the explicit form of G_0 we can show that

$$Q_0^{11}(E) = Q_0^{22}(E) = -\frac{m^*}{\pi\hbar^2}\left[\psi\left(\frac{1}{2} + t(E)\right) - \frac{\pi}{2}\mathrm{tg}\,(\pi t(E)) - \ln(2R) + C_E\right], \tag{3}$$

where $\psi(x)$ is the logarithmic derivative of the Γ-function, C_E is the Euler constant, and $t(E) = (2\hbar)^{-1}\sqrt{\hbar^2 + 2m^* R^2 E}$. The non-diagonal elements of $Q_0(E)$ have the form

$$Q_0^{12}(E) = Q_0^{21}(E) = -\frac{m^*}{2\hbar^2}\frac{1}{\cos(\pi t(E))}\mathcal{P}_{-\frac{1}{2}+t(E)}\left(-\cos(r_{12}/R)\right), \tag{4}$$

where $\mathcal{P}_\nu(x)$ is the Legendre function and $r_{12} = r(q_1, q_2)$. The transition amplitudes $S_{jk}(E)$ from the channel $\mathbf{R}_j^+$ to $\mathbf{R}_k^+$ at the energy level E and reflection amplitudes $S_{jj}(E)$ in the channel $\mathbf{R}_j^+$ forms the scattering matrix on the sphere $S(E)$. Using the Krein resolvent formula we can find as $S(E)$:

$$S = \left[\frac{i\hbar^2}{m^*}k + C + A^*\left(Q_0(E) - B\right)^{-1} A\right]\left[\frac{i\hbar^2}{m^*}k - C - A^*\left(Q_0(E) - B\right)^{-1} A\right]^{-1} \tag{5}$$

(here $k = \sqrt{2m^* E}/\hbar$ is the electron wave vector). Eq. (5) shows that the matrix B is just a matrix of parameters for a zero-range perturbation of H_0 at the points q_j; therefore, to avoid effects of non-locality we must choose B in a diagonal form: $\beta_{jk} = \delta_{jk}\beta_j$. It is known that the diagonal element β_j is expressed in terms of the scattering length $\lambda_j^{(0)}$ on the zero-range potential at the point q_j as follows: $\beta_j = -m^* \ln(\lambda_j^{(0)})/\pi\hbar^2$. The matrix C has a similar meaning, namely, C is a matrix of parameters for a zero-range perturbation of the free Hamiltonians in the wires. Thus, we must suppose C to be diagonal with the diagonal elements $\gamma_j = -m^*\lambda_j^{(1)}/\hbar^2$ where $\lambda_j^{(1)}$ is the scattering length for the zero-range potential at the point 0 in the wire $\mathbf{R}_j^+$. As to the matrix A, it is responsible for the transmission from the wires to the sphere. Indeed, if $A = 0$, then the transition coefficient $|S_{12}|^2 = |S_{21}|^2 = 0$. Eqs. (2) show that in the case of $\alpha_{jk} \neq 0$ for $j \neq k$ there are non-trivial boundary conditions which connect the wire $\mathbf{R}_j^+$ with the point q_k; therefore, we must suppose A to be diagonal, too. Moreover, the matrix $S(E)$ is symmetric only in the case of real elements $\alpha_{jj} \equiv \alpha_j$.

It is convenient to express these elements in terms of parameters λ_j having the dimension of length: $\alpha_j^2 = (m^*)^2\lambda_j/\hbar^2$. Thus, in our model the scattering on the sphere is described by means of the six real parameters $\alpha_j, \beta_j, \gamma_j$. Note, that in the case of a two-dimensional system, the zero-range perturbation vanishes in the limit $\beta_j \to \infty$; Eq. (5) shows that in this limit $S_{12}(E) \to 0$, as might be expected. We stress that the idealization of the one-dimensional wire is possible only in the case that the cross-section of the real wire is much less than the typical sizes of the system. In particular, our model works only in the case of relatively large distance r_{12}; namely, we shall suppose r_{12} is vastly larger than the Fermi wave length of an electron in the wire. Nevertheless, we can get the proper limit ($|S_{12}(E)| \to 1$ as $r_{12} \to 0$) using more general boundary conditions than those in (2).

2. Results and discussion

For reasons of symmetry we shall suppose $\gamma_1 = \gamma_2 \equiv \gamma$ and denote $\lambda_j^{(1)}$ simply by λ. In this case Eq. (5) gives the transition coefficient $T_{12}(E) = |S_{12}(E)|^2$ in the following form:

$$T_{12}(E) = \frac{(16k)^2\lambda_1\lambda_2\,|\widetilde{Q}_0^{12}|^2}{\left|4\lambda_1\lambda_2k^2 - 2ik(4 - ik\lambda)(\lambda_2\widetilde{Q}_0^{11} + \lambda_1\widetilde{Q}_0^{22}) - (4 - ik\lambda)^2\det\widetilde{Q}\right|^2}, \tag{6}$$

where $\widetilde{Q}(E)$ is the dimensionless Q-matrix: $\widetilde{Q}(E) = (\hbar^2/m^*)(Q(E) - B)$. Using Eq. (6) we can find the conductance G as a function of the chemical potential μ at temperature T. Namely, according to the Landauer–Büttiker formula

$$G(\mu, T) = \frac{2e^2}{\hbar^2}\int_0^\infty T_{12}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE, \tag{7}$$

where f_0 is the Fermi distribution function.

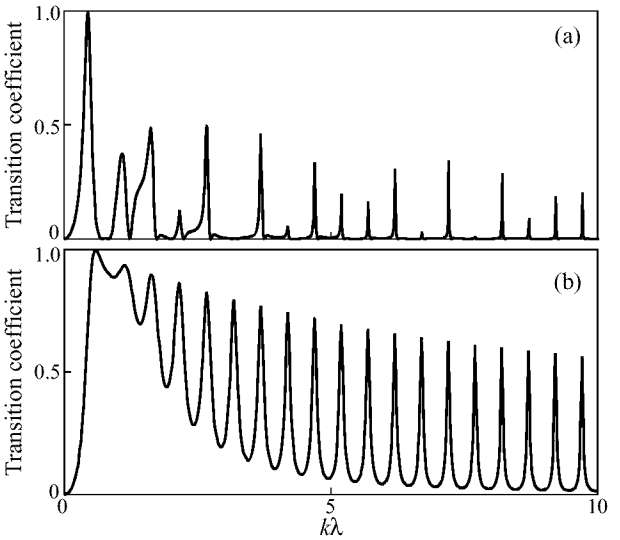

Fig. 1. Transition coefficient T_{12} as a function of $k\lambda$ ($k = \sqrt{2m^*E}/\hbar$): (a) case of a generic position for wires ($r_{12} = \sqrt{\pi}R$); (b) case of an antipodal position for wires ($r_{12} = \pi R$).

In the discussion, we restrict ourselves to the case of $\lambda_j = \lambda_j^{(0)} = \lambda$. The quantity T_{12} as a function of E has a series of sharp splash-like maxima, their positions are determined by the zeroes of $\det \widetilde{Q}(E)$, i.e., by the levels of the zero-range perturbation of H_0 with parameters β_j. On the other hand, if $r_{12} \neq \pi R$, then $\det \widetilde{Q}(E)$ has poles of the second order at the points of the spectrum of H_0, i.e., at the energy levels $E_l = \hbar^2 l(l+1)/2m^* R^2$ of an electron on the sphere **S**, and Eq. (7) shows that $T_{12}(E_l) = 0$ (see Figure 1(a)). It follows from the numerical analysis that T_{12} depends only slightly on the parameters β and γ.

If the points q_1 and q_2 are antipodal ($r_{12} = \pi R$), then the behavior of T_{12} at points E_l changes drastically. Indeed, at $E = E_l$ the numerator and the denominator in Eq. (7) have a pole of the same order, hence, $T_{12}(E_l)$ does not vanish. Therefore, the oscillation minima are not positioned on abscissa but they lay on a curve of the form $T_{12} = k(ak^2 + bk + c)^{-1}$ (Figure 1(b)). In the region $l \gg 1$ the oscillation period Δk is practically constant: $\Delta k = R^{-1}$. A numerical analysis of the conductivity at finite temperature shows that with a rise of temperature the peaks are smoothed and their amplitudes are lowered.

Acknowledgements

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